Supporting Information for:

Peptide-Nanowire Hybrid Materials for Selective Sensing of Small Molecules

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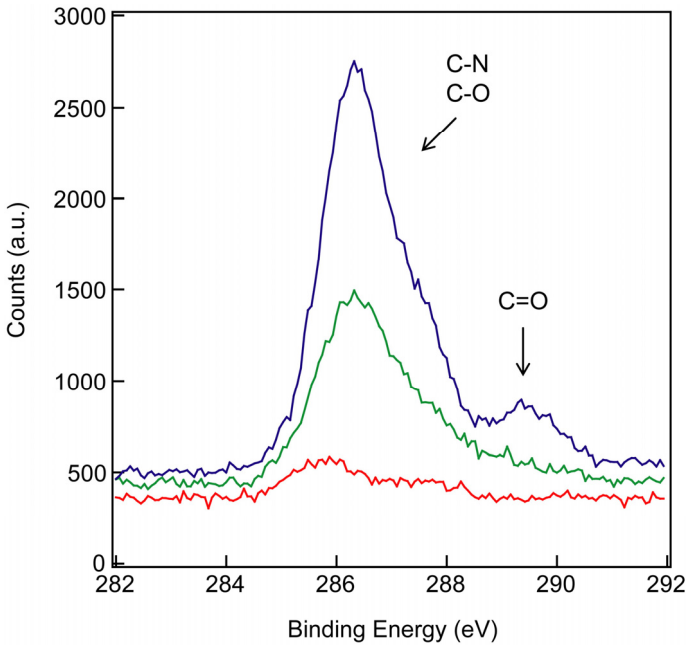

Figure S-1. Characterization of the bare silicon-on-insulator (SOI, red), amine-terminated (APTES, green), and peptide-coupled (blue) surfaces by X-ray photoelectron spectroscopy. Here, the C 1s region of the spectrum is shown.

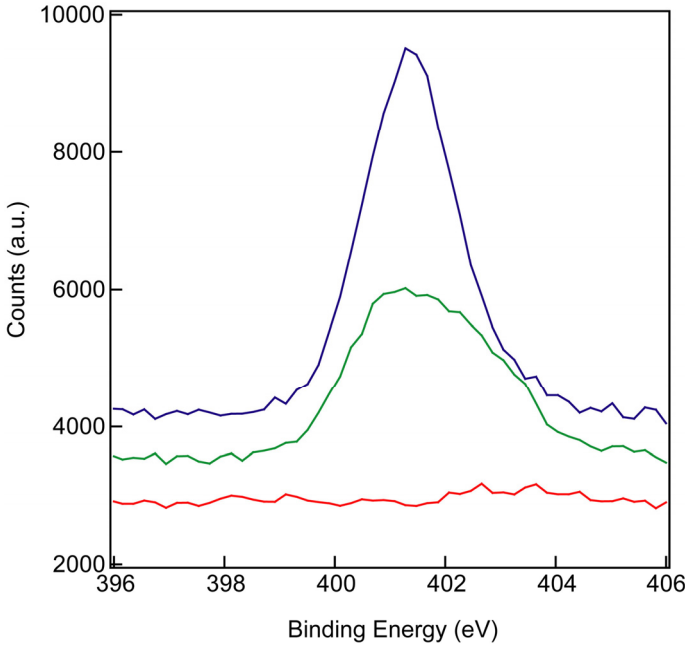

Figure S-2. Characterization of the bare silicon-on-insulator (SOI, red), amine-terminated (APTES, green), and peptide-coupled (blue) surfaces by X-ray photoelectron spectroscopy. Here, the N 1s region of the spectrum is shown.

Table S-1. Cartesian Coordinates (Angstroms) for the lowest conformation of the acetic acid binding peptide RVNEWVID. Force field (Dreiding) types are indicated. Charges are Mulliken population charges for the fully optimized geometry using B3LYP/6-31G**.

Atom	Dreiding Type	Charge	X	Y	Z
N1	N_3	-0.62304	-0.28671	5.85297	2.51909
H2	H___A	0.24676	-0.12212	6.86369	2.55669
H3	H___A	0.25680	0.10800	5.45007	3.37234
C4	C_3	0.06517	0.42076	5.29158	1.35036
H5	H_	0.07593	0.25932	4.21498	1.37348
C6	C_R	0.09738	-0.14085	5.85314	0.09249
O7	O_2	-0.31284	0.02146	7.07503	-0.13274
C8	C_3	-0.18912	1.95111	5.53560	1.46008
H9	H_	0.11684	2.31368	5.04832	2.36728
H10	H_	0.10328	2.13654	6.60837	1.54983
C11	C_3	-0.12359	2.74282	4.98807	0.24781
H12	H_	0.08896	2.43480	5.52276	-0.65381
H13	H_	0.08634	2.50816	3.93262	0.11378
C14	C_3	-0.08960	4.26815	5.14227	0.41835
H15	H_	0.15703	4.61593	4.53773	1.25888
H16	H_	0.14446	4.49587	6.18670	0.64551
N17	N_R	-0.27381	4.93986	4.78254	-0.79147
H18	H___A	0.30252	5.11528	5.50445	-1.42047
C19	C_R	0.01581	5.30883	3.53187	-1.16048
N20	N_R	-0.39336	5.91650	3.35859	-2.34948
H21	H___A	0.31200	6.08474	4.10802	-2.94117
H22	H___A	0.31722	6.19048	2.47216	-2.64075
N23	N_R	-0.37727	5.09216	2.43799	-0.40534
H24	H___A	0.37282	4.65967	2.49433	0.45688
H25	H___A	0.31106	5.36197	1.56205	-0.72372
N26	N_R	-0.40580	-0.79357	5.15341	-0.86699
H27	H___A	0.33144	-1.00123	5.64440	-1.68035
C28	C_3	0.01296	-1.17437	3.76652	-0.81347
H29	H_	0.16286	-1.61406	3.57868	0.16877
C30	C_R	0.10426	0.01939	2.89986	-0.97573
O31	O_2	-0.38264	0.80305	3.10065	-1.93236
C32	C_3	0.04600	-2.27341	3.41755	-1.86745
H33	H_	0.05530	-1.86988	3.60157	-2.86717
C34	C_3	-0.33737	-3.53490	4.29635	-1.69082
H35	H_	0.11515	-3.28889	5.34990	-1.82522
H36	H_	0.12176	-4.28454	4.02611	-2.43589
H37	H_	0.08922	-3.95700	4.15905	-0.69395
C38	C_3	-0.33531	-2.71028	1.93370	-1.79651
H39	H_	0.10133	-1.86377	1.28321	-2.02045
H40	H_	0.11448	-3.08887	1.69300	-0.80189
H41	H_	0.09025	-3.49213	1.73549	-2.53115
N42	N_R	-0.32851	0.25408	1.89495	-0.10081

H43	H___A	0.31910	-0.41765	1.71584	0.57739
C44	C_3	0.07073	1.40349	1.04274	-0.14208
H45	H_	0.12043	2.26949	1.61513	-0.48145
C46	C_R	0.06912	1.16996	-0.07592	-1.08069
O47	O_2	-0.31746	0.13733	-0.76822	-0.93954
C48	C_3	-0.13244	1.72596	0.46950	1.26213
H49	H_	0.10156	2.61835	-0.15283	1.19659
H50	H_	0.15109	0.89880	-0.16462	1.58126
C51	C_R	0.10466	1.96261	1.50245	2.28362
O52	O_2	-0.33285	2.96569	2.24303	2.20178
N53	N_R	-0.46142	1.13103	1.66889	3.32515
H54	H___A	0.29552	0.34279	1.11314	3.42892
H55	H___A	0.28437	1.31744	2.35433	3.98610
N56	N_R	-0.34843	2.05744	-0.38382	-2.05486
H57	H___A	0.33393	2.84003	0.18132	-2.14977
C58	C_3	0.06309	1.90034	-1.49916	-2.94784
H59	H_	0.11169	0.90509	-1.39522	-3.38943
C60	C_R	0.10141	1.92147	-2.83585	-2.29173
O61	O_2	-0.28823	1.51835	-3.81248	-2.96552
C62	C_3	-0.20349	2.90636	-1.44038	-4.13272
H63	H_	0.10103	2.78987	-0.48318	-4.64656
H64	H_	0.09672	2.62499	-2.21929	-4.84494
C65	C_3	-0.13836	4.40390	-1.65130	-3.78047
H66	H_	0.09710	4.94004	-1.91750	-4.69248
H67	H_	0.13623	4.50795	-2.48064	-3.07956
C68	C_R	0.16549	5.05557	-0.46073	-3.22073
O69	O_2	-0.50175	5.52945	-0.48051	-2.06471
O70	O_2	-0.37764	5.14352	0.59184	-3.88929
N71	N_R	-0.32087	2.32693	-3.02964	-1.01258
H72	H___A	0.30888	2.65477	-2.26213	-0.52040
C73	C_3	0.03651	2.25714	-4.28797	-0.32638
H74	H_	0.13754	2.29946	-5.08385	-1.07544
C75	C_R	0.07802	0.95959	-4.44664	0.37700
O76	O_2	-0.30357	0.38167	-5.55323	0.27599
C77	C_3	-0.11300	3.48982	-4.52346	0.58789
H78	H_	0.12289	4.38908	-4.42478	-0.02310
H79	H_	0.08651	3.46246	-5.55230	0.95295
C80	C_R	-0.13380	3.60277	-3.62092	1.75189
C81	C_R	-0.00382	2.97850	-3.79601	2.98677
H82	H_	0.12645	2.36555	-4.57547	3.23392
C83	C_R	-0.00661	4.35274	-2.45319	1.86389
N84	N_R	-0.28745	3.31055	-2.77695	3.79907
H85	H___A	0.28197	3.00517	-2.66222	4.71386
C86	C_R	0.00678	4.13715	-1.94822	3.14273
C87	C_R	-0.11427	5.20092	-1.79215	0.96681
H88	H_	0.11998	5.36763	-2.16275	0.03020

C89	C_R	-0.12908	4.74325	-0.75961	3.56403
H90	H_	0.09685	4.57461	-0.38983	4.50049
C91	C_R	-0.07893	5.82507	-0.60668	1.38403
H92	H_	0.09266	6.45591	-0.11823	0.74700
C93	C_R	-0.13595	5.59224	-0.08909	2.66986
H94	H_	0.09650	6.04736	0.77863	2.95733
N95	N_R	-0.30427	0.38583	-3.44298	1.08612
H96	H___A	0.29339	0.86699	-2.60323	1.15218
C97	C_3	-0.00160	-0.90866	-3.52256	1.70178
H98	H_	0.13208	-1.33932	-4.49495	1.45434
C99	C_R	0.07609	-1.78904	-2.49184	1.09785
O100	O_2	-0.30315	-1.54366	-1.27779	1.28875
C101	C_3	0.03592	-0.82578	-3.48397	3.25941
H102	H_	0.10229	-0.14238	-4.28389	3.55617
C103	C_3	-0.33279	-0.27476	-2.16937	3.86212
H104	H_	0.10634	-0.98823	-1.35603	3.72602
H105	H_	0.10033	-0.09711	-2.30043	4.93035
H106	H_	0.10537	0.66630	-1.89788	3.38686
C107	C_3	-0.33259	-2.19519	-3.80427	3.90183
H108	H_	0.09870	-2.56244	-4.76622	3.54088
H109	H_	0.10310	-2.09687	-3.85735	4.98709
H110	H_	0.10638	-2.92499	-3.03205	3.65091
N111	N_R	-0.28962	-2.83866	-2.86007	0.32687
H112	H___A	0.30282	-3.03120	-3.80854	0.24387
C113	C_3	0.02372	-3.68209	-1.94250	-0.38746
H114	H_	0.14067	-3.25309	-0.94072	-0.31193
C115	C_R	0.09794	-5.02841	-1.85988	0.23317
O116	O_2	-0.30412	-5.34287	-2.66178	1.14373
C117	C_3	-0.02846	-3.75404	-2.29933	-1.90888
H118	H_	0.07418	-4.39184	-1.55346	-2.38933
C119	C_3	-0.14376	-4.37876	-3.69848	-2.18418
H120	H_	0.08826	-5.24538	-3.84174	-1.53599
H121	H_	0.08587	-3.65240	-4.48073	-1.95289
C122	C_3	-0.32699	-2.35688	-2.17336	-2.56491
H123	H_	0.12416	-1.66255	-2.90220	-2.14173
H124	H_	0.09866	-2.42316	-2.33541	-3.64060
H125	H_	0.10675	-1.95781	-1.17309	-2.39864
C126	C_3	-0.35856	-4.85989	-3.88198	-3.63798
H127	H_	0.11051	-4.01751	-3.83849	-4.32915
H128	H_	0.10276	-5.34310	-4.85476	-3.73997
H129	H_	0.11858	-5.57936	-3.10371	-3.89811
N130	N_R	-0.30986	-5.91476	-0.92021	-0.17245
H131	H___A	0.30215	-5.63277	-0.29869	-0.86576
C132	C_3	0.00991	-7.24697	-0.78862	0.34559
H133	H_	0.16733	-7.43644	-1.59494	1.05854
C134	C_R	0.27118	-8.27381	-0.93822	-0.70893

O135	O_2	-0.25042	-7.96549	-1.06711	-1.91549
C136	C_3	-0.14421	-7.39399	0.54717	1.12238
H137	H_	0.14720	-6.58555	0.62735	1.85072
H138	H_	0.15280	-8.33627	0.52528	1.67335
C139	C_R	0.25035	-7.37745	1.75466	0.28324
O140	O_2	-0.27407	-8.39020	2.48536	0.22003
O141	O_R	-0.40339	-6.27354	2.09610	-0.41564
O142	O_R	-0.41160	-9.58231	-0.94241	-0.36942
H143	H___A	0.32294	-6.27549	2.90425	-0.97101
H144	H___A	0.33223	-10.27224	-1.04085	-1.05971

Table S-2. Cartesian Coordinates (Angstroms) for the lowest conformation of the ammonia binding peptide DLESFLD. Force field (Dreiding) types are indicated. Charges are Mulliken population charges for the fully optimized geometry using B3LYP/6-31G**.

Atom	Dreiding Type	Charge	X	Y	Z
N1	N_3	-0.63693	2.93094	7.60588	3.90474
H2	H___A	0.25818	3.59623	8.25893	4.33429
H3	H___A	0.35374	1.11783	9.11068	3.11243
H4	H___A	0.28106	2.98861	6.74721	4.46163
C5	C_3	0.06890	3.40069	7.29855	2.53511
H6	H_	0.14113	2.76721	6.51245	2.10814
C7	C_R	0.04415	4.80532	6.81992	2.54304
O8	O_2	-0.31401	5.71657	7.56855	2.97706
C9	C_3	-0.17219	3.26126	8.55739	1.64897
H10	H_	0.12985	3.84516	8.41996	0.73743
H11	H_	0.12090	3.65119	9.42940	2.17193
C12	C_R	0.22834	1.87529	8.82485	1.25357
O13	O_R	-0.45826	0.91237	9.09893	2.15615
O14	O_2	-0.25277	1.56579	8.80664	0.04481
N15	N_R	-0.30710	5.16483	5.62336	2.01889
H16	H___A	0.30857	4.48171	5.05780	1.61353
C17	C_3	0.03438	6.49217	5.10574	2.10367
H18	H_	0.13259	6.91624	5.38365	3.07405
C19	C_R	0.09065	7.33840	5.72206	1.08277
O20	O_2	-0.30289	7.60457	5.14766	-0.00032
C21	C_3	-0.18858	6.52844	3.56376	2.01599
H22	H_	0.12213	7.56516	3.22688	1.89042
H23	H_	0.08843	5.96156	3.27258	1.12557
C24	C_3	0.03562	5.88194	2.87554	3.24821
H25	H_	0.07129	4.84660	3.22080	3.34889
C26	C_3	-0.34880	5.85264	1.36459	2.99672
H27	H_	0.08904	5.30046	1.13796	2.08221
H28	H_	0.09935	6.87440	0.99095	2.90098
H29	H_	0.12247	5.35127	0.86392	3.82849
C30	C_3	-0.32856	6.62526	3.13206	4.58290

H31	H_	0.10048	7.69715	3.23951	4.40970
H32	H_	0.09843	6.27143	4.06932	5.02051
H33	H_	0.09832	6.44928	2.31292	5.29625
N34	N_R	-0.32307	7.84486	6.92851	1.40231
H35	H___A	0.29874	7.37811	7.39453	2.13228
C36	C_3	0.06703	8.92327	7.53573	0.70787
H37	H_	0.13233	9.58257	6.73253	0.34778
C38	C_R	0.07770	9.80669	8.39471	1.53976
O39	O_2	-0.30119	10.95799	8.63179	1.11721
C40	C_3	-0.22579	8.30239	8.19369	-0.53026
H41	H_	0.14589	7.32315	7.74337	-0.73495
H42	H_	0.12128	8.93685	7.97338	-1.38776
C43	C_3	-0.14295	8.09131	9.70605	-0.38712
H44	H_	0.12981	9.03355	10.22598	-0.26354
H45	H_	0.13703	7.45432	9.92345	0.46780
C46	C_R	0.25364	7.40637	10.17366	-1.57308
O47	O_2	-0.26475	6.34319	9.67021	-1.97847
O48	O_R	-0.42607	7.91703	11.14325	-2.34343
N49	N_R	-0.31973	9.47123	8.89633	2.74644
H50	H___A	0.29911	8.54394	8.95694	2.95814
C51	C_3	0.02846	10.44525	9.13044	3.76594
H52	H_	0.14353	11.37942	9.47764	3.29010
C53	C_R	0.12859	10.72720	7.81646	4.41326
O54	O_2	-0.30503	9.94910	7.30546	5.25235
C55	C_3	0.04017	10.01934	10.24944	4.74444
H56	H_	0.11570	9.12091	9.98366	5.32549
H57	H_	0.10763	9.80967	11.15886	4.17308
O58	O_3	-0.52463	11.12436	10.46342	5.61509
H59	H___A	0.31088	11.08962	11.37796	5.99535
N60	N_R	-0.34399	11.85183	7.21673	3.98181
H61	H___A	0.30145	12.31244	7.74946	3.29509
C62	C_3	0.06317	12.53649	6.00695	4.30198
H63	H_	0.13761	13.13055	6.28347	5.18272
C64	C_R	0.08264	13.55171	5.81180	3.21907
O65	O_2	-0.30998	14.33661	6.77530	3.06605
C66	C_3	-0.15079	11.67041	4.79252	4.74844
H67	H_	0.14930	10.89859	5.14177	5.43649
H68	H_	0.09269	12.34846	4.18703	5.34944
C69	C_R	-0.06074	11.01953	3.84806	3.80998
C70	C_R	-0.12959	10.76052	4.07616	2.44769
H71	H_	0.11640	10.91650	5.00316	2.04137
C72	C_R	-0.10563	10.63525	2.61305	4.35373
H73	H_	0.12862	10.80570	2.41617	5.34437
C74	C_R	-0.14373	10.27539	3.04121	1.62181
H75	H_	0.10994	10.22580	3.16938	0.60451
C76	C_R	-0.12562	10.06011	1.62374	3.55268

H77	H_	0.10636	9.80092	0.72953	3.96870
C78	C_R	-0.09056	9.90224	1.81398	2.18020
H79	H_	0.10687	9.54977	1.04624	1.59467
N80	N_R	-0.29059	13.69798	4.75869	2.36507
H81	H___A	0.29867	13.05030	4.01584	2.42344
C82	C_3	0.02708	14.73445	4.72823	1.33206
H83	H_	0.14909	15.52740	5.43154	1.61283
C84	C_R	0.09266	14.17594	5.26004	0.04264
O85	O_2	-0.31732	13.19631	4.68711	-0.48126
C86	C_3	-0.17934	15.49596	3.35192	1.24907
H87	H_	0.12170	15.99924	3.18371	2.20369
H88	H_	0.08688	16.28967	3.44097	0.49983
C89	C_3	0.02674	14.62273	2.10807	0.91149
H90	H_	0.07852	13.58857	2.42994	0.75443
C91	C_3	-0.35080	15.12341	1.44423	-0.39074
H92	H_	0.10131	14.45248	0.63356	-0.68866
H93	H_	0.10244	15.12355	2.18342	-1.19627
H94	H_	0.10943	16.13242	1.04436	-0.27117
C95	C_3	-0.32973	14.62460	1.05449	2.04595
H96	H_	0.10181	13.83493	0.32002	1.84882
H97	H_	0.09968	15.59567	0.56361	2.13604
H98	H_	0.10144	14.36626	1.55356	2.98164
N99	N_R	-0.29414	14.64673	6.38001	-0.57570
H100	H___A	0.31030	15.44454	6.80144	-0.18209
C101	C_3	-0.00785	14.01013	7.04679	-1.70641
H102	H_	0.16510	13.18868	6.41233	-2.05699
C103	C_R	0.27906	14.88348	7.27451	-2.90535
O104	O_2	-0.25046	16.08578	6.91911	-2.90844
C105	C_3	-0.14386	13.36877	8.38852	-1.21011
H106	H_	0.16191	12.72217	8.19872	-0.34810
H107	H_	0.15775	12.74536	8.78914	-2.01155
C108	C_R	0.25008	14.33805	9.44909	-0.89400
O109	O_2	-0.26501	14.53074	9.90831	0.25029
O110	O_R	-0.41411	15.03908	9.99468	-1.89563
O111	O_R	-0.41113	14.45269	7.93501	-4.01482
H112	H___A	0.32473	7.40470	11.41341	-3.13524
H113	H___A	0.32807	15.74364	10.70335	-1.78774
H114	H___A	0.33324	15.04638	8.14793	-4.75820

Table S-3. Cartesian Coordinates (Angstroms) for the reaction of the GLU4-ARG1 motif of RVNEWVID with acetic acid.

Reactants:

Atom	X	Y	Z
N1	0.00000	0.00000	0.00000
H2	0.00000	0.00000	1.02033

H3	0.98494	0.00000	-0.26908
C4	-0.59956	1.25176	-0.49903
H5	-1.62714	1.30435	-0.13116
C6	0.22967	2.42209	0.02872
O7	1.35777	2.62842	-0.41925
C8	-0.63592	1.21033	-2.03649
H9	-1.34139	0.42246	-2.32128
H10	0.35049	0.90254	-2.40395
C11	-1.00531	2.55044	-2.68605
H12	-0.13363	3.20850	-2.66187
H13	-1.77868	3.04937	-2.09990
C14	-1.49256	2.41421	-4.13216
H15	-2.47049	1.92190	-4.16333
H16	-0.81139	1.79490	-4.72345
N17	-1.58100	3.70037	-4.83107
H18	-0.74754	4.00094	-5.31561
C19	-2.44855	4.69125	-4.52662
N20	-2.26995	5.90941	-5.05158
H21	-1.41683	6.14072	-5.54514
H22	-2.83621	6.70888	-4.70831
N23	-3.50654	4.47003	-3.76066
H24	-3.67714	3.58350	-3.29942
H25	-4.11091	5.28191	-3.51849
N26	-0.22627	3.14679	1.08996
H27	0.39051	3.90942	1.34387
C28	-1.58726	3.24525	1.58030
H29	-1.97500	2.26756	1.88100
C30	-2.53480	3.91435	0.57604
O31	-2.09727	4.58826	-0.34774
N32	-3.85971	3.69033	0.75589
H33	-4.17370	3.31354	1.64144
C34	-4.83140	4.34474	-0.09350
H35	-4.30551	4.56779	-1.02099
C36	-5.28835	5.67087	0.53734
O37	-5.40901	5.77941	1.76115
C38	-6.00694	3.41024	-0.40771
H39	-6.74451	3.97034	-0.99615
H40	-6.50761	3.09178	0.51195
C41	-5.57007	2.22361	-1.25695
O42	-4.74729	2.34885	-2.16613
N43	-6.15393	1.03926	-0.98308
H44	-6.86243	0.93838	-0.27198
H45	-5.94732	0.24188	-1.57142
N46	-5.49465	6.64171	-0.35309
H47	-5.36237	6.46590	-1.36230
C48	-5.77527	8.03398	-0.05690

H49	-5.60862	8.18838	1.01161
C50	-4.86493	8.98070	-0.85972
H51	-3.81912	8.75464	-0.62841
H52	-5.05034	9.99435	-0.48752
C53	-5.05096	9.01176	-2.39552
H54	-4.61192	9.93657	-2.77321
H55	-6.12445	9.03963	-2.62102
C56	-4.41758	7.86111	-3.18849
O57	-4.86327	6.68238	-2.96886
O58	-3.53481	8.12485	-4.03723
H59	-6.82726	8.26200	-0.25747
H60	-1.55860	3.85274	2.48438
C61	-1.18019	9.71414	-5.91444
C62	-0.79989	8.63402	-6.87115
O63	-1.05583	8.95093	-8.14839
H64	-0.79881	8.19223	-8.70532
H65	-0.37490	9.83516	-5.19266
H66	-1.39230	10.65766	-6.41666
H67	-2.06069	9.39554	-5.34526
O68	-0.31531	7.55508	-6.56353

Products:

Atom	X	Y	Z
N1	0.00000	0.00000	0.00000
H2	0.00000	0.00000	1.01997
H3	0.98476	0.00000	-0.26882
C4	-0.61607	1.24169	-0.50537
H5	-1.65852	1.24961	-0.17650
C6	0.15193	2.43486	0.06772
O7	1.21015	2.80459	-0.44061
C8	-0.60652	1.22588	-2.03437
H9	-1.19937	0.35785	-2.34508
H10	0.41849	1.04501	-2.37916
C11	-1.13717	2.50235	-2.70275
H12	-0.37704	3.28604	-2.63752
H13	-2.02710	2.87843	-2.18473
C14	-1.46716	2.23914	-4.18204
H15	-2.46643	1.80380	-4.28228
H16	-0.76567	1.50121	-4.58398
N17	-1.37866	3.40262	-5.05735
H18	-0.47589	3.59026	-5.47192
C19	-2.38065	4.22529	-5.41613
N20	-2.19294	5.05649	-6.44308
H21	-1.41765	4.89449	-7.06993
H22	-2.91475	5.77267	-6.71268
N23	-3.55672	4.21327	-4.79187

H24	-3.64993	3.90094	-3.82704
H25	-4.28786	4.86143	-5.16061
N26	-0.28150	2.99451	1.22931
H27	0.28831	3.77321	1.54230
C28	-1.57735	2.86177	1.86737
H29	-2.00158	1.87259	1.69824
C30	-2.51937	3.98374	1.43010
O31	-2.10166	5.14274	1.37782
N32	-3.78674	3.64721	1.12974
H33	-4.09813	2.69392	1.27052
C34	-4.77969	4.65134	0.73947
H35	-4.24149	5.39948	0.15402
C36	-5.33967	5.30210	2.02548
O37	-6.42844	4.98058	2.49449
C38	-5.89543	4.04919	-0.10029
H39	-6.68147	4.80377	-0.21387
H40	-6.37531	3.21656	0.42570
C41	-5.46729	3.61680	-1.49687
O42	-4.33427	3.81730	-1.93691
N43	-6.42466	3.00598	-2.22167
H44	-7.38429	2.95728	-1.90801
H45	-6.24132	2.78832	-3.19147
N46	-4.51028	6.19396	2.60428
H47	-3.57620	6.26034	2.20630
C48	-4.70058	6.66023	3.97605
H49	-4.50401	5.84034	4.67888
C50	-3.78052	7.83833	4.29412
H51	-2.75331	7.58937	4.00442
H52	-3.76904	7.97956	5.37788
C53	-4.18851	9.15561	3.63143
H54	-4.36361	9.04369	2.55801
H55	-3.37981	9.89069	3.73116
C56	-5.40486	9.77701	4.27699
O57	-5.75529	9.58961	5.42379
O58	-6.06524	10.60399	3.44971
H59	-5.75049	6.93327	4.10803
H60	-1.44019	2.96213	2.94934
C61	-6.23307	7.82268	-7.04249
C62	-5.14501	6.82780	-6.66218
O63	-5.44514	5.95126	-5.80610
H64	-6.80672	10.99198	3.95156
H65	-5.90971	8.51001	-7.82617
H66	-7.12765	7.28666	-7.37515
H67	-6.52267	8.40100	-6.15858
O68	-4.01938	6.93990	-7.21829

Table S-4. Cartesian Coordinates (Angstroms) for the reaction of the deprotonated aspartic acid ASP1 and the N-terminus motif of DLESFLD with ammonia.

Reactants:

Atom	X	Y	Z
N1	0.00000	0.00000	0.00000
H2	0.00000	0.00000	1.02126
H3	3.23282	0.00000	-2.87317
H4	-0.97937	0.08419	-0.27117
C5	0.53092	-1.28316	-0.45818
H6	0.34159	-1.37232	-1.53130
C7	-0.11226	-2.46367	0.28078
O8	-0.26816	-2.42075	1.50392
C9	2.05043	-1.35073	-0.20517
H10	2.40491	-2.37200	-0.39082
H11	2.26471	-1.11250	0.83891
C12	2.88583	-0.44283	-1.06969
O13	2.63036	-0.59088	-2.38244
O14	3.74232	0.30938	-0.65209
N15	-0.46427	-3.52578	-0.46466
H16	-0.36669	-3.53486	-1.47019
H17	-0.85884	-4.34191	-0.01331
N18	1.34480	2.27166	-1.74822
H19	1.36296	1.76835	-2.63440
H20	2.31867	2.31658	-1.45066
H21	0.89418	1.62580	-1.08823

Products:

Atom	X	Y	Z
N1	0.00000	0.00000	0.00000
H2	0.00000	0.00000	1.02304
H3	3.50410	0.00000	0.09505
H4	-0.52987	0.82981	-0.26528
C5	-0.73981	-1.20618	-0.41365
H6	-1.21319	-1.02420	-1.38278
C7	-1.81704	-1.57094	0.61090
O8	-1.69699	-1.25703	1.79745
C9	0.22005	-2.39735	-0.59958
H10	-0.35582	-3.32936	-0.59808
H11	0.92313	-2.44372	0.23788
C12	0.94324	-2.32183	-1.95601
O13	0.21111	-2.30303	-2.96777
O14	2.21618	-2.29402	-1.94754
N15	-2.86577	-2.27808	0.15337
H16	-2.98483	-2.49795	-0.82536
H17	-3.57732	-2.58973	0.80209

N18	2.86390	0.00309	-0.70017
H19	3.17180	0.71226	-1.36697
H20	2.82731	-0.94744	-1.16504
H21	1.87612	0.18940	-0.39287

Table S-5. Energetics for the various combinations of ammonia and acetic acid with DLESFLD and RVNEWVID peptide binding motifs (from Tables S-3 and S-4). Absolute energies are in Hartrees, while reaction energies are in kcal/mol.

Reactions	Reactants Hartrees	Products Hartrees	ΔE kcal/mol
Ammonia binding peptide			
DLESFLD + NH_3 → $DLESFLD^-$ + NH_4^+	-549.05088	-549.06260	-7.40
DLESFLD + CH_3COOH → $DLESFLD^+$ + CH_3COO^-	-721.58317	-721.58248	0.43
DLESFLD + $N(CH_3)_3$ → $DLESFLD^-$ + $NH(CH_3)_3^+$	-666.95796	-666.97832	-12.78
Acetic acid binding peptide			
RVNEWVID + NH_3 → $RVNEWVID^-$ + NH_4^+	-1573.88215	-1573.85801	15.15
RVNEWVID + CH_3COOH → $RVNEWVID^+$ + CH_3COO^-	-1746.37934	-1746.38817	-5.54